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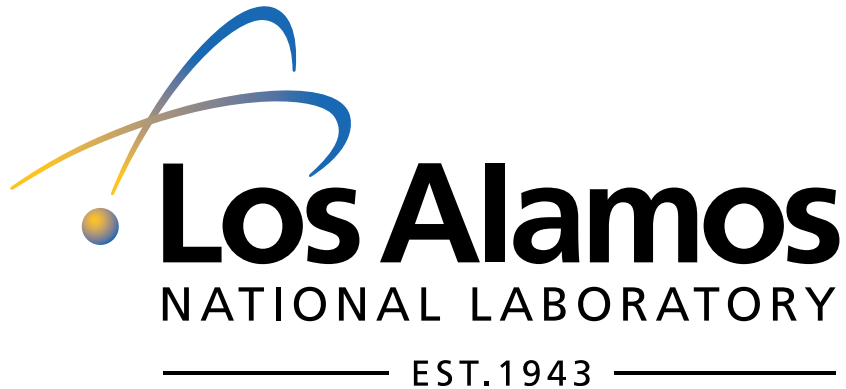|	
Title:	Los Alamos Applied Energy Programs
Author(s):	Guthrie, George Drake Jr. Fox, Melissa Miller
Intended for:	Various briefings
Issued:	2020-11-02

DEPARTMENT OF ENERGY

Office of the Secretary

Dan Brouillette
Secretary

Vacant
Deputy Secretary

- Inspector General (IG)
- Federal Energy Regulatory Commission (FERC)
- Ombudsman
- Chief of Staff

Boards and Councils

Office of the Under Secretary for Nuclear Security and National Nuclear Security Administration (NNSA)

Administrator, NNSA

Principal Deputy Administrator, NNSA

- Deputy Administrator for Defense Programs (NA-10)
- Deputy Administrator for Defense Nuclear Nonproliferation (NA-20)
- Deputy Administrator for Naval Reactors (NA-30)
- Associate Administrator for Emergency Operations (NA-40)
- Associate Administrator for Safety, Infrastructure & Operations (NA-50)
- Chief & Associate Administrator for Defense Nuclear Security (NA-70)
- Associate Administrator for Counter-Terrorism & Counter-Proliferation (NA-80)
- Associate Administrator for External Affairs (NA-EA)
- Associate Administrator for Management & Budget (NA-MB)
- Associate Administrator for Acquisition & Project Management (NA-APM)
- Office of General Counsel (NA-GC)
- Associate Administrator for Information Management & Chief Information Officer (NA-IM)

Office of the Under Secretary for Science (S4)

Under Secretary for Science

Deputy Under Secretary for Science

- Office of Science (SC)
- Office Artificial Intelligence and Technology (AI)
- Office of Technology Transitions (OTT)
- Assistant Secretary for Environmental Management (EM)
- Office of Legacy Management (LM)
- National Laboratory Operations Board

Office of the Under Secretary of Energy (S3)

Under Secretary of Energy

- Assistant Secretary for Cybersecurity, Energy Security & Emergency Response (CR)
- Office of Policy (OP)
- Indian Energy Policy & Programs (IE)
- Loan Programs Office (LPO)
- Associate Under Secretary for Environment, Health, Safety and Security (AU)
- Office of Project Management Oversight and Assessments (PM)

- Assistant Secretary for Fossil Energy (FE)
- Assistant Secretary for Nuclear Energy (NE)
- Assistant Secretary for Energy Efficiency & Renewable Energy (EERE)
- Assistant Secretary for Electricity (OE)
  - Bonneville Power Administration (BPA)
  - Southeastern Power Administration (SEPA)
  - Southwestern Power Administration (SWPA)
  - Western Area Power Administration (WAPA)

- U.S. Energy Information Administration (EIA)
- Assistant Secretary for International Affairs (IA)
- Office of Enterprise Assessments (EA)
- Office of General Counsel (GC)
- Office of the Chief Human Capital Officer (HC)
- Office of Management (MA)
- Office of Intelligence and Counterintelligence (IN)

- Advanced Research Projects Agency – Energy (ARPA-E)
- Assistant Secretary for Congressional & Intergovernmental Affairs (CI)
- Office of Public Affairs (PA)
- Office of the Chief Financial Officer (CF)
- Office of the Chief Information Officer (IM)
- Office of Small & Disadvantaged Business Utilization (OSDBU)
- Office of Economic Impact & Diversity (ED)
- Office of Hearings & Appeals (HG)

Updated 1/13/2020

Los Alamos Contributes to DOE Energy Programs

Energy Efficiency and Renewable Energy (EERE)

- Vehicle Technologies
- Bioenergy Technologies
- Hydrogen and Fuel Cells Technologies
- Geothermal Technologies
- Wind Energy Technologies
- Advanced Manufacturing

Advanced Research Projects Agency-Energy (ARPA-E)

Transformational energy projects

Office of Electricity (OE)

- Advanced Grid Research & Development
- Energy Storage
- Microgrid Research & Development
- Grid Modernization Laboratory Consortium

Cybersecurity, Energy Security, and Emergency Response (CESER)

- Cybersecurity for Energy Delivery Systems
- Infrastructure Security & Energy Restoration

Office of Fossil Energy (OFE)

- Carbon Storage
- Carbon Capture
- Unconventional Technologies
- Advanced Energy Systems
- Cross-cutting Research (rare-earth elements; materials in extreme conditions)

Applied Energy Multi-institutional Partnerships

National Risk Assessment Partnership

Carbon Capture Simulation for Industry Impact

Producing Algae for Coproducts and Energy

Electrocatalysis Consortium

Fuel Cell Performance and Durability

Grid Modernization Laboratory Consortium

In turn, our participation in partnerships supports and enriches the Lab's multidisciplinary capabilities

Energy Efficiency and Renewable Energy Portfolio

- **Bioenergy**
  - **Advanced Algae Systems:** Algae as a bio-feedstock for fuels and bioproducts; molecular tools to improve growth and productivity
  - **Feedstock and Logistics**: Addressing woody biomass and corn stover processing bottlenecks
  - **Conversion**: Technologies for conversion into biofuels, bioproducts, and biopower synthesis
  - **Advanced Development and Optimization:** Integrating individual technologies into a system/process
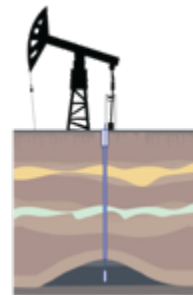
- **Vehicle Technologies**
  - Developing an internal combustion model—FEARCE code helps engine designers understand combustion processes

- **Fuel Cells**
  - Polymer Electrolyte Membrane (PEM) technology
  - Focus on fundamental understanding for materials and process development – PGM-free catalysts, alkaline membranes, and enhancing durability of fuel cell components

Crude oil

Fuel Cell Stack
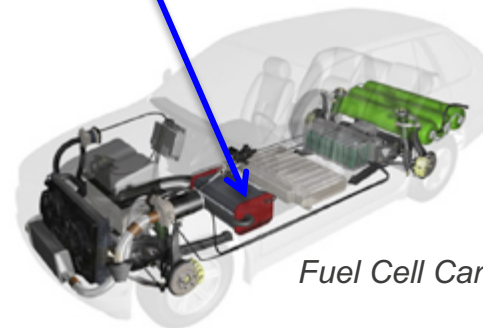
Fuel Cell Car

DOE Plastics Innovation Challenge
A comprehensive DOE program to accelerate innovations in energy-efficient plastics

Bio-**O**ptimized **T**echnologies for keeping **T**hermoplastics out of the **L**andfill and **E**nvironment (BOTTLE)

LANL Effort
Use high throughput screening approaches to enable the rapid identification of new/improved enzymes for plastic deconstruction and upcycling

- Deconstruction (Task Co-lead): Focus on *bio-based* deconstruction of plastics (nylon, polyurethanes)
- Upcycle & Redesign: Enzyme and strain improvement, co-design with new polymers
- Participate in the leadership team

LANL Capabilities Leveraged
Computational protein design, strain and enzyme evolution, biosensor development

Delivering robust processes to upcycle existing waste plastics, and develop new plastics and processes that are recyclable-by-design

Partners: NREL · OAK RIDGE National Laboratory · Los Alamos National Laboratory · MONTANA STATE UNIVERSITY · MIT Massachusetts Institute of Technology · Colorado State University
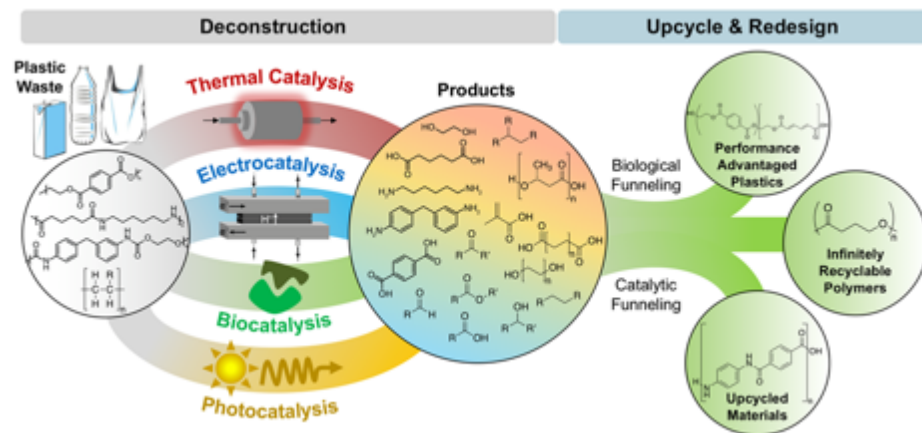
Technical and Strategic Leadership in BOTTLE

Technical and Consortium Leadership
Taraka Dale, B-11

- High throughput screening expertise
- Strategic planning
- Structuring objectives, tasks, milestones
- R&D prioritization

Technical Leadership
Ramesh Jha, B-11

- Computational protein engineering
- Biosensor design and development
- High-throughput screening to enable plastic waste deconstruction and to improve its bioconversion into higher-value product
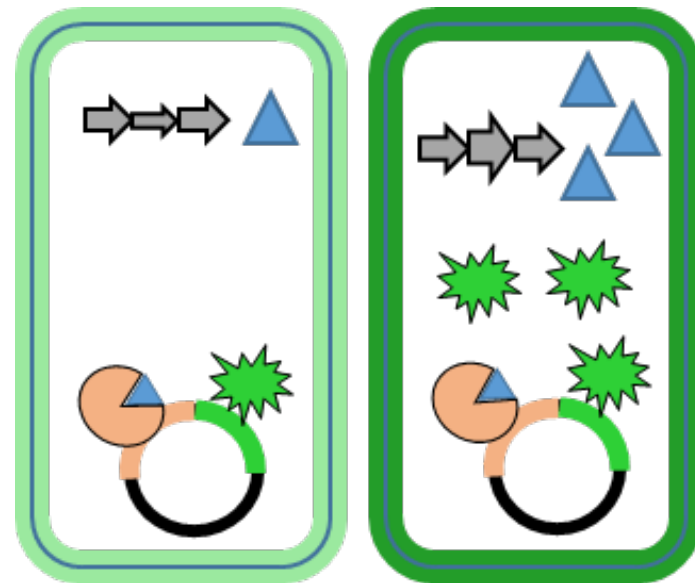
LANL's Smart Microbial Cell Technology will be used to rapidly report on deconstruction products and to improve new microbes for biological funneling and upcycling to new products.

Technical and Strategic Leadership in HFTO Consortia

Fuel Cell Performance and Durability (FC-PAD)
Rodney Borup, MPA-11, Director

- Enhancing the performance and durability of polymer electrolyte membrane fuel cells while simultaneously reducing their cost
- Goal is to demonstrate world-class improvements in fuel cell performance and durability that exceed the targets set by the U.S. DOE
- Currently being re-competed as M2FCV (Million Mile Fuel Cell Vehicle), $10M/yr for 5 years (LANL and LBNL co-lead)

Electrocatalysis (ElectroCat)
Co-Director: Piotr Zelenay, MPA-11

- Accelerating the development and deployment of platinum group metal-free (PGM-free) electrocatalysts in fuel cells
- Employs a systematic approach in which potential catalysts are synthesized and analyzed rapidly and comprehensively using high-throughput, combinatorial methods
- Currently being re-competed as ElectroCat 2.0, $3M/yr for 3 years (LANL and ANL co-lead)

Energy Efficiency and Renewable Energy Portfolio

- **Geothermal**
  - 3D seismic images reveal vertically oriented faults and fractures to help determine optimal locations for drilling
  - 3D acoustic imaging beyond the borehole for real-time monitoring of wellbore integrity
  - Machine learning applied to geothermal systems **3 new projects funded in FY19**
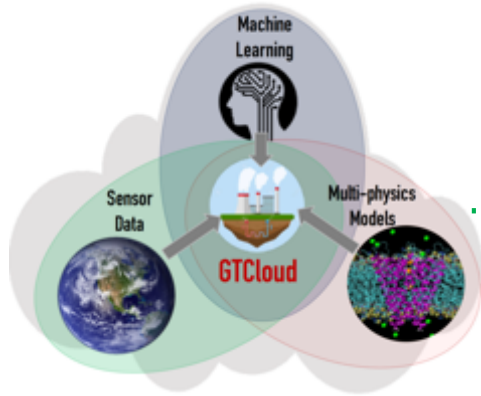
- **Advanced Characterization of State of Stress, Critical Stress, and Permeability in Geothermal Systems Applying Machine Learning** (Paul Johnson, EES-17, $500K)

- **Cloud Fusion of Big Data and Multi-Physics Models Using Machine Learning for Discovery, Exploration and Development of Hidden Geothermal Resources** (Monty Vesselinov, EES-16, $500K)

- **Detecting and Characterizing Fracture Zones Using a Convolutional Neural Network** (Lianjie Huang, EES-17, $200K)

- **Wind**
  - HPC code enables high resolution simulations of complex atmospheric and turbine blade interactions with the goal of increasing turbine reliability, performance and optimal placement

Fossil Energy Portfolio

- **Carbon Storage**
  - Predicting the integrity of seals and wellbores
  - Multi-phase subsurface flow and transport modeling and prediction
  - Novel methods to detect small leaks over large areas
    - seismic and acoustic imaging coupled with machine learning
 - Monitoring for faults at a critical state of stress
- **Oil & Gas**
  - Modeling flow in fractured systems
  - Prediction of fracture networks
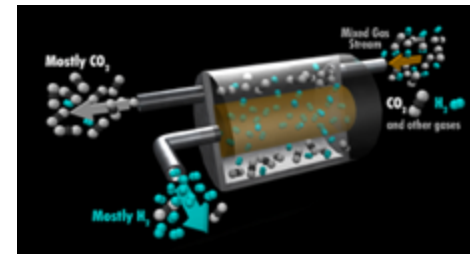 - Physics-based analysis of production
- **Carbon Capture**
  - Pre-combustion membrane separations
  - Carbon Capture Simulation Initiative
    - New computational tools and models to enable industry to more rapidly develop and deploy new advanced energy technologies
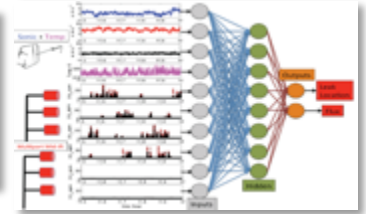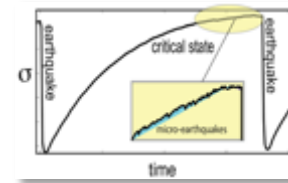
Extracting Small Signals in Real Time
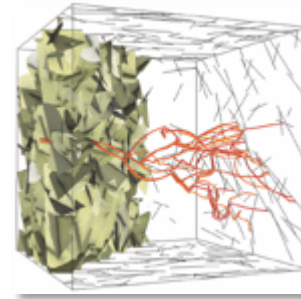
Flow in Fractured Systems

Membrane and Module Design, Evaluation, and Scale-Up

SMART Initiative is developing novel machine-learning applications to transform subsurface decisions.

- **New initiative targets improving real-time decisions for subsurface**
  - Combines accuracy and predictability of physics with speed of machine learning

- **New challenges in fossil energy parallel challenges in national-security mission**
  - New signature identification (small signals, noisy background)
  - Rapid prediction for complex, uncertain systems

- **10-year initiative, launched in summer 2019**
  - Initial (proof-of-concept) phase—2 years, ~$20M from both FE-20 & FE-30
  - Oil/gas—Improve decisions on recovery & economics for fractured reservoirs (e.g., shales)
  - CO_2—Improve decisions on monitoring & operations of CO_2 storage

Technical and Strategic Leadership in SMART

Strategic and Technical and Leadership
George Guthrie, SPO-AE

- Detail with DOE-FE and NETL to develop strategy and technical vision for initiative
- Serves on SMART Advisory Board

Technical Leadership
Rajesh Pawar, EES-16

- Lead for multi-organizational team focused on virtual learning for CO_2 storage
- LANL lead for SMART-CS

Technical Leadership
Hari Viswanathan, EES-16

- Lead for multi-organizational team focused on virtual learning for shale-gas
- LANL lead for SMART-OG

Fossil Energy Portfolio - Crosscutting Research

- **Rare Earth Elements**
  - Establish alternate sources of rare earth elements (REE) to reduce dependence on foreign supply
    - No domestic production since 2016
    - Majority of mining/production from China
  - Demonstrate the ability to use advanced dissolution techniques to leach REE from fly ash.
  - Develop and test the ability to use advanced dissolution techniques and solvent extraction contactors to extract REE from coal-related materials
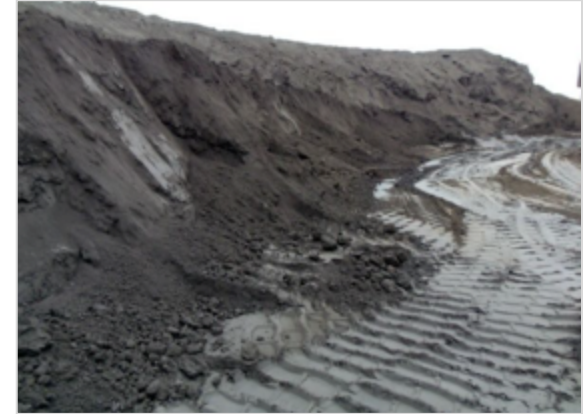
Fly ash, a solid by-product from burning coal, is investigated as an alternative REE resource

- **Extreme Environment Materials**
  - eXtremeMAT will result in toolsets that address gaps in current physics-based materials modeling, data analytics, and machine learning
  - Reliable prediction of materials performance over long service lifetimes in fossil energy power plant environments

eXtremeMAT Strategic and Technical Leadership

Founding Strategic Leadership
David Teter, MST

- Strategic leader of XMAT since inception; thought leader of overall program
- Developed relations with external stakeholders; harmonized interests of the various national laboratory partners
- Served as Chair of the the XMAT Stakeholder Advisory Board

**Current Technical and Strategic Leadership**
Laurent Capolungo, MST-8

- Lead author of XMAT 5-year plan, including technical direction, tasks, and technical objectives
- Leads work scoping for technical teams across national labs for all of XMAT
- Task 2 (modeling and simulation) technical lead
- Stakeholder engagement, budget and strategy planning, active participant on the XMAT Stakeholder Advisory Board
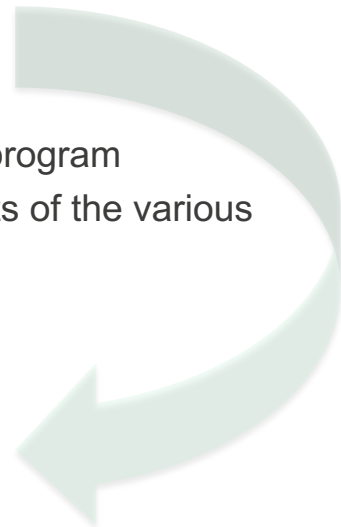
eXtremeMAT Wins and New Partnerships

Quick Win: New Modeling Capability

- Predicts likelihood of material failure, differs from existing ASME type approaches (no uncertainty)
- Allows optimization of structural designs and rapid certification of new materials
- Considers materials aging, stress and temperature cycling
    - Demonstration to DOE-FE of applicability
    - Leveraged past work part of DoE NE-NEAMS and added new capabilities
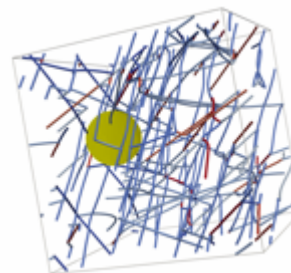   - Significant interest from Siemens and Southern Company to test LANL models
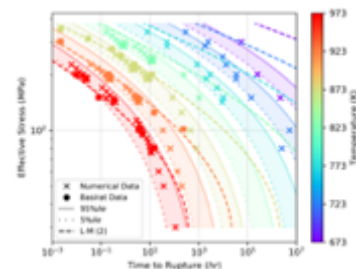
XMAT's new rupture life model for P91

New Partnership with UTRC ![United Technologies Research Center]

- HPC4 Materials project uses LANL models to extrapolate potential response of a new material ($300K/year)

Simulation of cavity nucleation in the presence of defects

XMAT Attracts New Talent

Nathan Bieberdorf (UC Berkeley) received a 2019 LANL Distinguished Student Award for his contributions

Aaron Kohnert, early career staff scientist in MST, leads the development of damage nucleation models

Office of Electricity Portfolio

- **Advanced Grid Modeling**
  - **Integrated Control and Optimization Under Uncertainty**
    - Develop new algorithms and models to mitigate the effects of uncertainty on electrical power systems and natural gas pipelines
  - **Interdependent Energy Networks**
    - Understand the propagation of stress, dynamics, uncertainty, and prices across power/gas networks to enable optimal operations
    - Apply physics-inspired machine learning to difficult power systems applications
  - **Design of Resilient Power Systems**
    - Optimize design, hardening, and resilience upgrades of power systems to withstand and recover from extreme events
  - **Analysis of Extreme Events and Threats**
    - Independent, science-based evaluation of threats to infrastructure

- **Energy Storage**
  - **Non-aqueous Flow Batteries**
    - Develop flow batteries that are more scalable and flexible for grid scale energy storage – pursuing Fe and all organic
    - Increase energy density by increasing voltage per redox couple and overall decrease the cost of flow cells

*"LANL researchers are also **providing key input into critical infrastructure protection**…That work, in turn, will inform our Defense Critical Electric Infrastructure (DCEI) efforts."*

Bruce Walker, Assistant Secretary, Office of Electricity

LANL LEADERSHIP

A collaboration between DOE, national labs, and industry, the NAERM will ultimately provide real-time situational awareness and analysis capabilities for emergency events for optimal operations and recovery

- LANL's work on **modeling**, especially on the natural gas side, will inform the NAERM and future investments

- LANL researchers are providing key input into **critical infrastructure protection**

- This work will **inform Defense Critical Electric Infrastructure (DCEI) efforts**

Leveraging and Building Upon National Lab Research Investments
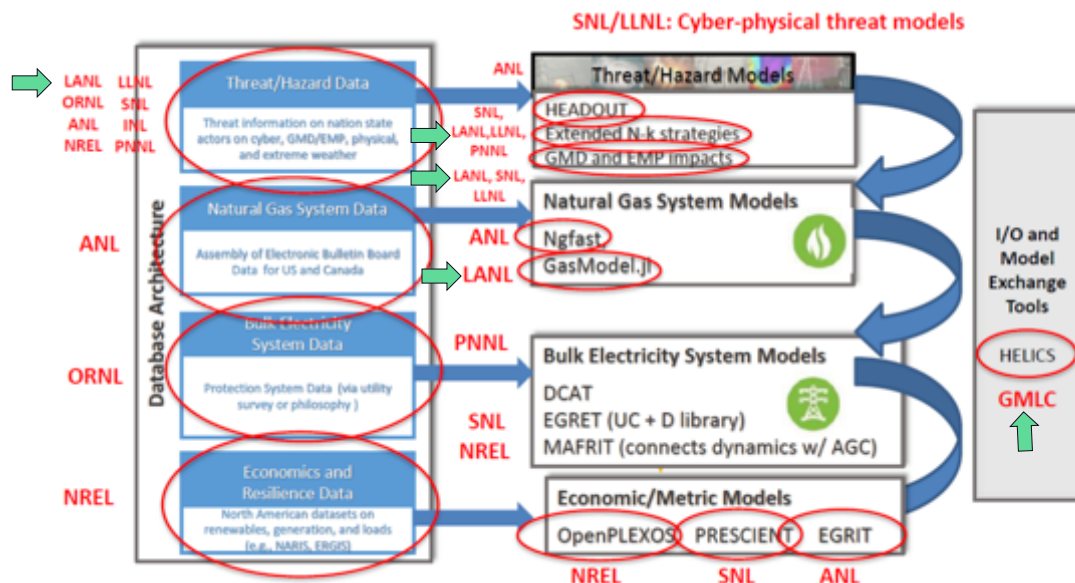
NAERM Technical Leadership

Strategic and Technical Leadership

Russell Bent, T-5

- Contributed to DOE vision for NAERM
- LANL Co-chair of the NAERM natural gas domain
- Validation and verification of NAERM models

NAERM Software Framework
Delivered September 2019

Natural Gas Hydraulic Modeling Capability
To be delivered September 2020

NAERM leverages LANL capabilities in infrastructure science to address gas modeling needs

- **GasModels.jl developed at LANL**
    - Enables computational evaluation of emerging gas network formulations and algorithms in a common platform

- **OE funded project**
    - Efficient infrastructure utilization—improve deliverability of natural gas
    - Gas market design and analysis-–value-driven delivery of natural gas

advanced network science initiative (ansi)

Defense Critical Electric Infrastructure (DCEI)

- **LANL selected to develop a small scale microgrid on site to demonstrate resiliency**

- Once hardware is installed, tests will be run to demonstrate that the microgrid is functional

- If successful, this demo will be an example for other DCEI sites, and OE will likely want to bring others (DoD) on site to demonstrate

- LANL is partnering with other labs on proposals for providing modeling tools that can assess vulnerabilities and, ultimately, develop prioritized mitigation strategies for DCEI sites
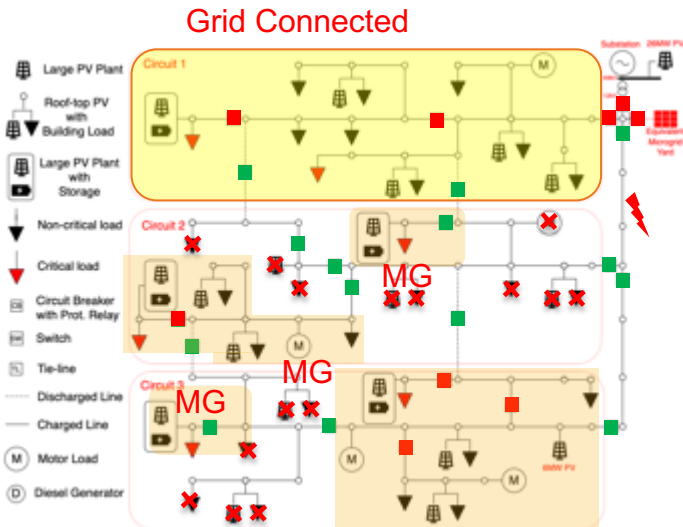
Resilient Operations of Networked Microgrids (Russell Bent, PI)

- Funded by DOE Microgrid Research and Development Program

- Objective: Improve resiliency of power systems with optimization-based methods

- Outcome: First-of-kind, high-fidelity physics-based optimization method for modeling networked microgrids

- LANL capabilities developed in this program will be leveraged for DCEI

Cybersecurity, Energy Security, and Emergency Response (CESER) Portfolio

- **Cyber Security for Energy Delivery Systems (CEDS)**
  - Algorithms for optimal grid design to minimize the impact of cyber-physical attacks on the power grid
  - Software and hardware to integrate Quantum Communication Transceivers and secure communications between locations

- **Infrastructure Security and Energy Restoration (ISER)**
  - Data analytics and modeling to deliver a catalog of historical weather-related outage events– this information is integrated into EAGLE-I reports
  - Electromagnetic Pulse/Geomagnetic Disturbance - modeling and assessing the effects of E3 waveforms on the electric power system
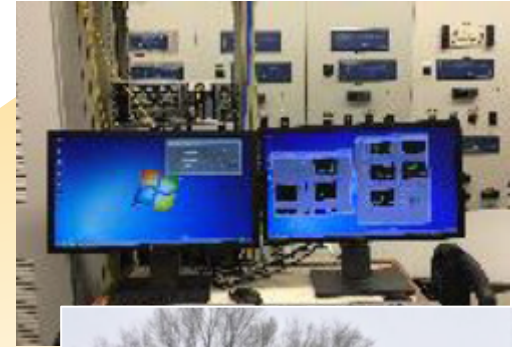
*Preliminary testing on LANL electric grid **successful**; sustained operation over 13 days, including 40-inch snowfall.*

# Emerging Opportunities in CEDS

Technical Leadership
Ray Newell, P-21

- Technical lead on LANL quantum key distribution (QKD) capability
- LANL lead in partnership with EPB to demonstrate effectiveness of QKD as means of secure communications for the nation's electricity suppliers

Analysis on the Wire (AoW) Project (led by BNL)

- As part of the Computational Science Initiative (CSI), the AOW project is building a prototype platform for in-network computing

- Possible applications for the smart grid (e.g. real/near-real time load forecasting and state estimation)

- Security is a challenge that could be addressed by leveraging LANL's miniaturized QKD capability, in combination with MDI-QKD technology from ORNL

- Potential new project will couple these developments together with Stony Brook's room temperature quantum memories to develop a viable, implementable solution
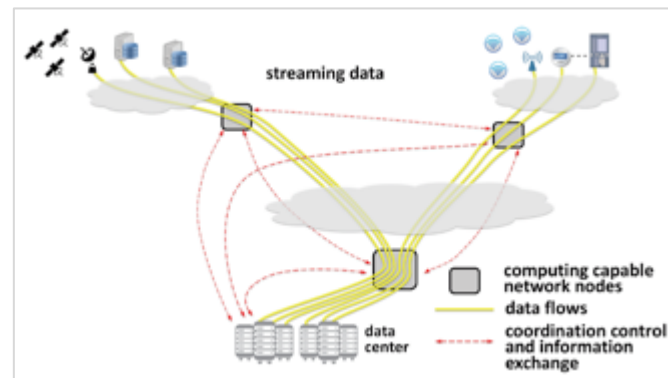
Security challenge: AoW nodes have to be privy to encryption keys to decrypt and process this data

Recent Growth in Our ARPA-E Portfolio

2018 OPEN

Advanced Manufacturing of Embedded Heat Pipe Nuclear Hybrid Reactor

DV Rao, PI; $4.5M total; $2.5M LANL
Partners: Westinghouse, U-Pitt, INL

Stable Diacid Coordinated Quaternary Ammonium Polymers for 80-150°C Fuel Cells

Yu Seung Kim, PI; $3.5 M total; $1.8M LANL
Partners: Toyota, UNM, RPI

Making Demand-Response Work for a More Stable, Secure Energy Grid

Drew Geller, PI; $600K LANL
Lead: U. Michigan

2018 MEITNER

Self-regulating, Solid Core Block for a Walk-away Safe Heat Pipe Reactor

DV Rao, LANL PI; $2.4M LANL
Lead: Westinghouse

2019 TOPICS

Portable Neutron and Soft X-ray Diagnostics for Transformative Fusion-Energy Concepts

Glen Wurden, PI; $630K LANL
Partners: University of Nevada-Reno

2019 DIFFERENTIATE

Machine Learning Based Well Design to Enhance Unconventional Energy Production

Monty Vesselinov, PI; $2.4M total; $1.3M LANL
Partners: MIT, Stanford, UNM, Julia Computing

2020 BETHE

**Target Formation and integrated Experiments for Plasma-Jet Driven Magneto-Inertial Fusion**

Samuel Langendorf, PI; $4.6M total; $1.9M LANL
Partners: HyperJet Fusion Corporation, UNM, UAH, and Virginia Tech and State University

Electromagnetic & Particle Diagnostics for Transformative Fusion-Energy Concepts

Glen Wurden, PI; $375K total; $300K LANL
Partners: University of Nevada-Reno

Applied Energy Portfolio: Essential, Exciting, Impactful

Four of the 11 LANL 2019 R&D 100 Awards entries reflect innovation and collaboration in support of the national ENERGY SECURITY mission
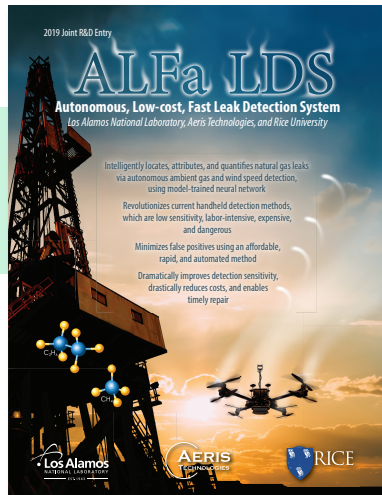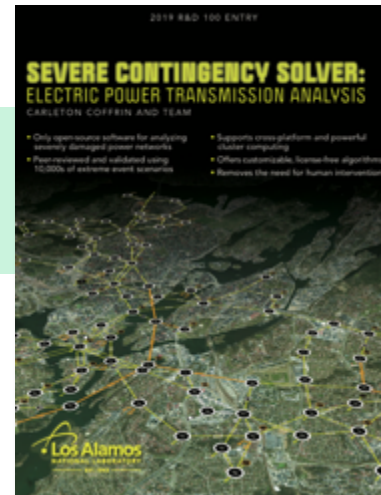

System intelligently locates, attributes, and quantifies natural gas leaks

Funded in part by ARPA-E

Software for engine designers to develop higher efficiency, lower emission vehicles

Funded by EERE

Software analyzes severely damaged electric power networks

Funded by Office of Electricity

Software enables infrastructure design for CO_2 capture, transport, storage

Funded by Office of Fossil Energy